

Butanoic acid, propyl ester
105-66-8 | DTXSID6059318

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -84.3 °C

Global applicability domain: Inside

Local applicability domain index: 9.92e-01

Confidence level: 7.98e-01

Nearest Neighbors from the Training Set

Image not found

Butanoic acid, propyl ester

Measured: -95.2

Predicted: -84.3

Image not found

Butyl propionate

Measured: -89.0

Predicted: -84.2

Image not found

Ethyl valerate

Measured: -91.2

Predicted: -83.8

Image not found

Pentyl acetate

Measured: -70.8

Predicted: -83.2

Image not found

Methyl hexanoate

Measured: -71.0

Predicted: -82.6